Bell inequalities and entanglement at quantum phase transition in the XXZ Model

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Entanglement and violation of Bell inequalities are aspects of quantum nonlocality that have been often confused in the past. It is now known that this equivalence is only true for pure states. Even though almost all the studies of quantum correlations at quantum phase transitions only deals with entanglement, we here argue that Bell inequality can also reveal a general quantum phase transition. This is also shown for a particular case of two spin-$\frac{1}{2}$ in an infinity one dimensional chain described by the XXZ model. In this case, the Bell inequality is able to signal not only the first order phase transition, but also the infinity order Kosterlitz-Thouless quantum phase transition, which can not revealed neither by the energy of the system nor by the bipartite entanglement. We also show that, although the nearest-neighbors spins are entangled they, unexpectedly, never violate the Bell inequality. This indicates that the type of entanglement which is relevant for quantum phase transition is not trivial, *i.e.*, can not be revealed by the Bell inequality.

I. INTRODUCTION

The concept of entanglement has evolved since it has first appeared in 1935, as a "spooky action at a distance", *i.e.*, the possibility of one system to influence another instantaneously, even at large distances [1]. Only in 1964, John Bell moved the concept from the philosophical debates to the laboratory, using inequalities - now known as Bell inequalities [2]. Entanglement was then a property of states which could not be described by realistic local theories. Perhaps the more drastic evolution of the concept came in 1989, with the work of R. F. Werner [3]. Werner defined entangled states as the ones which could not be created using local operations on the systems with classical communication between the parts; these operations may create only classical correlations. However, Werner surprisingly found mixed states which were entangled, according to his definition, but did not violate the Bell inequality. Entanglement and non-locality became distinct, but related, concepts.

Even though entanglement has all these facets, the word is usually used to designate quantum correlations that are "stronger" than classical ones. On the other hand, phase transitions (*e.g.*, magnetic phase) are generally related to an emerging order with origin in long range correlations. Quantum phase transitions (QPT) are the ones occurring at zero temperature, where the systems is in a pure quantum state. Therefore, we may expect these long range correlations to come from entanglement.

Studies trying to link entanglement and QPT first appeared in 2002 for specific models [4, 5]. Later, it was shown that, in principle, entanglement should inherit the non-analytical behavior of the ground state energy at any QPT; since both originate in the ground state [6, 7]. However, accidental non-analytical behavior may also appear, or disappear, due to the maximization process involved in entanglement definitions [8]. Nowadays, there are many studies concerning the link between entaglement and QPT. Their results can be favorable or unfavorable to it, depending of the specific model and the measurement of entanglement used (for a review see [9]). Nonetheless, to find such a link, all these studies used the Werner definition of entanglement and did not analyze non-local properties of the states.

In this work, we complement the study of the relation between entanglement and QPT, analyzing the non-local aspects of quantum phase transition using Bell inequalities. *The objective is to find: i) if entangled states, that may play a role in a quantum phase transition, are also non-local; ii) if the Bell Inequality is able to signal QPT.* We argue that, in principle, the Bell Inequality should also signal quantum phase transitions. A particular case of two spins in an infinite one-dimensional spin-$\frac{1}{2}$ XXZ Heisenberg chain was then studied. The study of non-local aspects of QPT is very recent, with only one analysis of a particular case of the one dimensional XY Heisenberg chain with a transverse magnetic field published[10][35].

In order to be self contained, we organize the article as follows: In Sec. II we give a brief introduction about entanglement and non-locality through Bell Inequality, highlighting its differences. Sec. III describes the XXZ model and its relevant quantities, in particular how to compute its correlation functions. The mathematical expression for the entanglement and Bell Inequalities in the specific case of the XXZ model are given in Sec. IV. The main results and a detailed discussion of their implications are in Sec. V and we conclude in Sec. VI.

II. ENTANGLEMENT AND NON-LOCALITY

Bell inequalities investigate correlations between two parties who share a quantum state. In the case of two spins 1/2 particles, each side, A and B, choose one direction, $\hat{a}_i$ and $\hat{b}_j$, and measures, simultaneously and independently, the observables $\mathbf{A_i} = \hat{a}_i.\sigma$ and $\mathbf{B_j} = \hat{b}_j.\sigma$; with $\sigma = (\sigma^x, \sigma^y, \sigma^z)$. If each part picks two directions, Bell inequalities state that any theory which is *both realistic and local* gives [36]

$$|\langle B_{CHSH}\rangle| = |\langle \mathbf{A_1} \otimes \mathbf{B_1}\rangle + \langle \mathbf{A_1} \otimes \mathbf{B_2}\rangle + \langle \mathbf{A_2} \otimes \mathbf{B_1}\rangle$$
$$- \langle \mathbf{A_2} \otimes \mathbf{B_2}\rangle| \le 2. \qquad (1)$$

The value obtained for $\langle B_{CHSH}\rangle$ depends both on the state and on the directions chosen. So, for a given state one should maximize over all directions defining a Bell measurement as:

$$\mathcal{B} = \max_{\{\hat{a}_i, \hat{b}_j\}} |\langle B_{CHSH}\rangle|. \qquad (2)$$

The states for which $\mathcal{B} > 2$ are the ones which cannot be described by a realistic local theory and were then associated with non-classical correlation or non-locality [37]. Clearly, states which can be written in a product or separable form, $|\phi_A\rangle|\phi_B\rangle$, are local. These states are known as separable or not entangled.

In 1989, Werner [3] proposed a definition of separability for mixed states from an operational point of view: separable states are the ones which can be produced by local operations and classical communication (LOCC). They can be written as

$$\rho_{AB} = \sum_k p_k \rho_A^{(k)} \otimes \rho_B^{(k)}, \qquad (3)$$

with $0 \le p_k \le 1$ and $\sum_k p_k = 1$. Separable mixed states can be correlated, but this correlation is a classical one that comes from the probabilities p_k. Surprisingly, in the same work, Werner constructed states which are entangled by his definition, but nonetheless do not violate the Bell inequality. Entanglement, although necessary, is not a sufficient condition for a mixed state to be nonlocal; Bell inequality does not capture all "kinds of entanglement".

For pure bipartite states, only in 1991, Gisin proved that entanglement is a necessary and sufficient condition for a state to be non-local [11]. Until nowadays, there are many attempts to draw a unifying picture between non-locality and entanglement by generalizing the Bell inequality. Popescu, in 1995, for example, showed that an entangled state not violating Bell, could be made to violate it after some processing with LOCC [12]. Another possibility, is to allow each part to make a measurement in a third direction. This originates a new inequality that is violated by states which do not violated CHSH inequality [13]. For a introduction and review on similar attempts see [14]. There are also many other definitions of non-locality, and all of them show some anomaly with entanglement [15]. For example, while for two qubits pure states the degree of violation of the Bell inequality is a increasing function of the entanglement of the state, this is not true for two qudits. Finally, there are also other definitions of quantum correlation, as the discord which has also been studied at quantum phase transitions [16–18].

III. SPIN-$\frac{1}{2}$ XXZ MODEL

We now describe the physics of the model we intend to use to study the relationship between entanglement and non-locality: an one dimensional spin-$\frac{1}{2}$ chain where the spins interact through anisotropic Heisenberg interaction. It is known as XXZ model and for N particles its Hamiltonian is given by

$$H = \sum_{j=1}^{N} [S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z], \qquad (4)$$

where $S_j^u = \sigma_j^u/2$ ($u = x, y, z$), σ_j^u are the Pauli spin-$\frac{1}{2}$ operators on site j, Δ is the anisotropy parameter, and $\sigma_{j+N}^u = \sigma_j^u$. The XXZ model cannot be diagonalized, but its energy spectrum can be obtained by Bethe ansatz. The Hamiltonian has two symmetries: i) a discrete parity $\mathbb{Z}_2$ symmetry over the plane xy: $\sigma^z \to -\sigma^z$, and ii) a continuous $U(1)$ symmetry that rotates the spins in the xz plane by any angle θ. The $\mathbb{Z}_2$ symmetry implies that $\langle \sigma_i^z\rangle = 0$ and $\langle \sigma_i^x \sigma_j^z\rangle = \langle \sigma_i^y \sigma_j^z\rangle = 0$, while the $U(1)$ symmetry implies that $\langle \sigma_i^x\rangle = \langle \sigma_i^y\rangle = 0$, $\langle \sigma_i^x \sigma_j^x\rangle = \langle \sigma_i^y \sigma_j^y\rangle$ and $\langle \sigma_i^x \sigma_j^y\rangle = 0$. However, in the thermodynamical limit a quantum phase transition occur and breaks the discrete $\mathbb{Z}_2$ symmetry; a continuous symmetry may not be broken at one-dimension even at zero temperature. The model has three phases:

i) $\Delta \le -1$: the system is in a ferromagnetic phase with all the spins pointing in the same direction. There is a first order quantum phase transitions (1QPT) at the critical point $\Delta = -1$.

ii) $-1 < \Delta < 1$: the system is in a gapless phase, where the correlation decays polynomially.

iii) $\Delta > 1$: the system is in the anti-ferromagnetic phase. The critical point at $\Delta = 1$ is of infinite order or Kosterlitz-Thouless quantum phase transitions (KT-QPT).

The Bethe ansatz solution gives the ground state energy [19, 20]:

$$e_0(\Delta) = \begin{cases} -\frac{\Delta}{4}, & \Delta \le -1, \\ \frac{\Delta}{4} + \frac{\sin \pi\nu}{2\pi} \int_{-\infty+\frac{i}{2}}^{\infty+\frac{i}{2}} dx \frac{1}{\sinh x} \frac{\cosh \nu x}{\sinh \nu x}, & -1 < \Delta < 1, \\ \frac{1}{4} - \ln 2, & \Delta = 1, \end{cases} \qquad (5)$$

where $\Delta = \cos \pi\nu$. For $\Delta > 1$ we just need to change $\nu = i\phi$ in (6).

The correlation functions, on the other hand, cannot be easily obtained from the Bethe ansatz solution. They are given in terms of very complicated multiple integrals, and solving them is a non trivial mathematical problem. However, for nearest neighbors we can obtain the correlation from $e_0(\Delta)$:

$$\langle \sigma_i^z \sigma_{i+1}^z\rangle = 4\frac{\partial e_0(\Delta)}{\partial \Delta}, \qquad (6)$$

$$\langle\sigma_i^x\sigma_{i+1}^x\rangle = \langle\sigma_i^y\sigma_{i+1}^y\rangle = \frac{1}{2}(4e_0(\Delta) - \Delta\langle\sigma_i^z\sigma_{i+1}^z\rangle). \quad (7)$$

For spins further apart, progress has been slow, but there are already some expressions available up to third neighbors [20]. We will not show them here, since they are too lengthy [38].

We are interested in the entanglement and non-local properties of two spins in the chain. These can be determined by the reduced density matrix of the two spins, which can be obtained from the magnetizations and correlations. Actually, the density matrix of any two spins-$\frac{1}{2}$can be expressed as

$$\rho_{i(i+r)} = \frac{1}{4}\left[\mathbb{I}\otimes\mathbb{I} + \mathbf{p}.\sigma\otimes\mathbb{I} + \mathbb{I}\otimes\mathbf{q}.\sigma + \sum_{u,v}t_r^{uv}\sigma_i^u\otimes\sigma_{i+r}^v\right],$$
$$(8)$$

with r being the distance between the sites, $\mathbf{p} = \langle\sigma\otimes\mathbb{I}\rangle$, $\mathbf{q} = \langle\mathbb{I}\otimes\sigma\rangle$, and $t_r^{uv} = \langle\sigma_i^u\sigma_{i+r}^v\rangle$. Due to the Hamiltonian symmetries, only $\{t_r^{xx}, t_r^{yy}, t_r^{zz}\}$ do not vanish and $t_r^{yy} = t_r^{xx}$. Translation invariance also implies that the correlation functions for two-sites depend only on the distance between the sites (r), being independent of i. So for the XXZ model we have

$$\rho_r = \frac{1}{4}\begin{pmatrix} 1+t_r^{zz} & 0 & 0 & 0 \\ 0 & 1-t_r^{zz} & 2t_r^{xx} & 0 \\ 0 & 2t_r^{xx} & 1-t_r^{zz} & 0 \\ 0 & 0 & 0 & 1+t_r^{zz} \end{pmatrix}. \quad (9)$$

Remark that in the ordered phases, ferro and antiferromagnetic, due to the spontaneous symmetry breaking (SSB), a finite value of the magnetization will emerge: $\langle\sigma_i^z\rangle = m$. This should be taken into account, complicating a little bit the expression for ρ. However, in many studies this is not done, and the simpler expression, preserving the symmetries, is used. In this case, the ground state used is not the one which breaks the symmetry and is stable against external perturbations, but a superposition of the two degenerated ground states with opposite magnetizations. This could be justified for the study of very small systems where the SSB does not happen, but not for real macroscopic systems. It is true, however, that all the thermodynamical quantities, which comes from the energy eigenvalues, are not affected by this choice. Nonetheless, entanglement properties may be affected by this choice, since it also depends on the eigenvectors [21, 22]. Last, besides the symmetric superposition of the two ground states, one could also think of an equiproportional mixture of the two, that would emerge if one takes the limit of temperature going to zero.

IV. BELL MEASUREMENT AND CONCURRENCE

In general, checking a Bell inequality violation is a high-dimensional variational problem. We have to optimize over the various possible measurements settings that each observer performs (see Eq. (2)). One simplification is that the value of B_{CHSH} and $\mathcal{B}$ does not depend on local properties, the magnetizations $\mathbf{p}$ and $\mathbf{q}$, but only on the correlations t^{uv}. For two spin-$\frac{1}{2}$ particles a closed analytic expression for the maximum violation of the Bell inequality was obtained by the Horodeckis [23] and is given in in terms of the matrix $U = T^T T$ by

$$\mathcal{B} = 2\sqrt{u + u'}, \quad (10)$$

with u and u' the two largest eigenvalues of U and T the 3×3 matrix build from the correlations t^{uv}. As u and u' are combinations of the correlation functions, we can rewrite it in terms of the correlations.

The expression for $\mathcal{B}$ in terms of the correlations is very cumbersome for general states. But, because of the symmetries of the XXZ model, see Eq. (9), it becomes quite simple. In fact, the matrix T is already diagonal, with t^{xx}, t^{yy} and t^{zz} as its diagonal elements and $t^{yy} = t^{xx}$. Therefore, the eigenvalues of U are $(t^{xx})^2$ and $(t^{zz})^2$ and we only have to check which is greater. The expression becomes

$$\mathcal{B}_r = 2\max\{\sqrt{2\langle\sigma_i^x\sigma_{i+r}^x\rangle^2}, \sqrt{\langle\sigma_i^x\sigma_{i+r}^x\rangle^2 + \langle\sigma_i^z\sigma_{i+r}^z\rangle^2}\}. \quad (11)$$

To have non-locality, we need either

- i)$|\langle\sigma_i^x\sigma_{i+r}^x\rangle| \geq |\langle\sigma_i^z\sigma_{i+r}^z\rangle|$ and $|\langle\sigma_i^x\sigma_{i+r}^x\rangle| > \frac{1}{\sqrt{2}}$

or

- ii)$|\langle\sigma_i^x\sigma_{i+r}^x\rangle| < |\langle\sigma_i^z\sigma_{i+r}^z\rangle|$ and $\langle\sigma_i^x\sigma_{i+r}^x\rangle^2 + \langle\sigma_i^z\sigma_{i+r}^z\rangle^2 > 1$.

To compare the non-locality with entanglement between the two spins, we will use the concurrence as our entanglement measure; see [24] for a review on entanglement measures. It is a well defined entanglement measure and is given in terms of the spectrum of $\rho\rho'$, where $\rho' = \sigma^y\otimes\sigma^y\rho^*\sigma^y\otimes\sigma^y$ is the time-reversed density matrix. Let λ_l be the eigenvalues of $\rho\rho'$ so that $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$. Then the concurrence is

$$\mathcal{C} = \max\{0, \sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}\}. \quad (12)$$

The concurrence can also be written in terms of the correlation functions, but in general the expression is also very cumbersome, since it comes from solving a polynomial of fourth degree. As in the case of the Bell inequality, due to the symmetries, for the XXZ model the expression is simple and given by [25]

$$\mathcal{C}_r = \max\left\{0, \frac{2|\langle\sigma_i^x\sigma_{i+r}^x\rangle| - (1 + \langle\sigma_i^z\sigma_{i+r}^z\rangle)}{2}\right\}. \quad (13)$$

As mentioned before, the Bell inequality is not directly affected by local properties, the magnetizations, but only depends on the correlations, given by the matrix T. The concurrence, however, may be affected, since the local magnetizations may appear in its expression. Eq. (13)

is only valid when the magnetizations and off-diagonal correlations are null ($\langle \sigma_i^\alpha \rangle = 0$ and $\langle \sigma_i^x \sigma_j^z \rangle = \langle \sigma_i^x \sigma_j^y \rangle = \langle \sigma_i^y \sigma_j^z \rangle = 0$), and no simple expression can be obtained in terms of the correlation for the general case. This may have consequences to the effect of the spontaneous symmetry breaking on these properties. In the case of the XXZ model, the SSB manifests itself with a finite value of $\langle \sigma_i^z \rangle$, which could in principle change the value of the concurrence, but not of the Bell inequality. However, as showed in [25], it turns out that for the XXZ model the concurrence does not change when the SSB is taken into account.

V. RESULTS

Before showing the results of non-locality and compare with the entanglement, let us look at the ground state energy per site e_0, as shown in Fig. 1. We can see the non-analytical behavior of $\frac{\partial e_0}{\partial \Delta}$ at the 1QPT $\Delta = -1$ and the nonexistence of non-analyticities at the KT-QPT at $\Delta = 1$. We also show the correlation functions for first, second and third neighbors in figs. 2 and 3. A non-analytical behavior can also be seen at $\Delta = -1$, and at least for first neighbors, it is directly related to the one found in e_0.
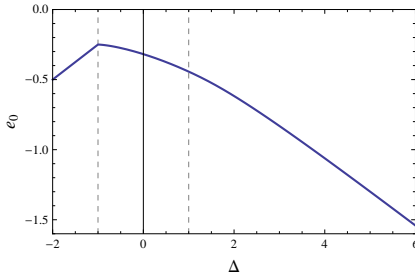

Figure 1: Ground state energy per site of the XXZ model as a function of the anisotropy Δ. There is a first order quantum phase transition at $\Delta = -1$ from a ferromagnetic to a gapless phase. At $\Delta = 1$ there is an infinite order Kosterlitz-Thouless phase transition from the gapless to the anti-ferromagnetic phase, which is not indicated by e_0.

Last, we review the results of the bipartite entanglement between two spins, first obtained in [26]. In Fig. 4 we observe that the entanglement of first neighbors suddenly appears as they enter the gapless phase, achieve the maximum at the KT-QPT, and slowly decrease in anti-ferromagnetic phase. Second and third neighbors are only slight entangled and in a small region on the right of the 1QPT; the curves can barely be seen in Fig. 4. The first order phase transition is indicated by the non-analytical behavior of the concurrence of all the first
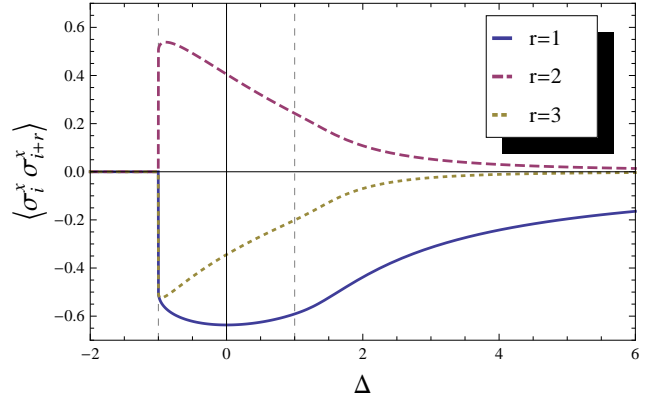

Figure 2: Correlation function in the $\hat{x}$ direction, $\langle \sigma_i^x \sigma_{i+r}^x \rangle$, for first, second and third neighbors of the XXZ model as a function of the anisotropy Δ. It can be seen that the correlation is able to signal the first order quantum phase transition at $\Delta = -1$, but not the infinite order quantum phase transition at $\Delta = 1$.
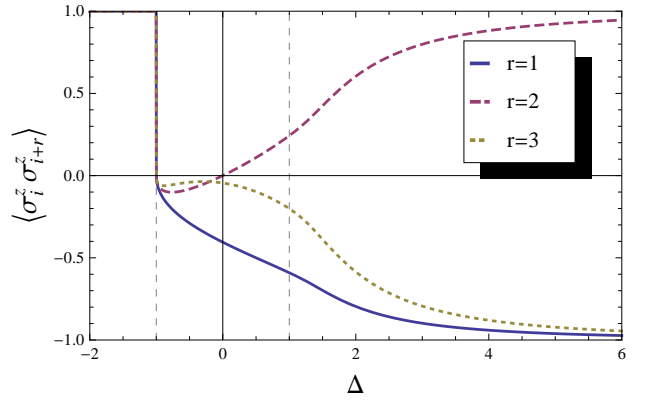

Figure 3: Correlation function in the $\hat{z}$ direction, $\langle \sigma_i^z \sigma_{i+r}^z \rangle$, for first, second and third neighbors of the XXZ model as a function of the anisotropy Δ. It can be seen that the correlation is able to signal the first order quantum phase transition at $\Delta = -1$, but not the infinite order quantum phase transition at $\Delta = 1$.

three neighbors: its first derivative diverges (see Fig. 6 for the case of first neighbors)

We now present our results. First we argue that the Bell Inequality may be as good as entanglement to signal the QPT. The argument is equivalent and follows directly from the one used in [6] for bipartite entanglement and in [27] for multipartite: for Hamiltonians with only nearest-neighbors interactions not only the entanglement between nearest-neighbors spins, but also e_0 can be obtained from the reduced density matrix of the two spins; they are functions of $\rho_{i,i+1}$. So any non-analytical behavior in $e_0 = f(\rho_{i,i+1})$ will also appear in the entanglement $E = g(\rho_{i,i+1})$, unless the the specific form of the functions f and g cause the non-analitycal behavior or originate accidental cancellations (see [8] for example). Note that while f is a linear function of $\rho_{i,i+1}$, g involves

the absolute value of $\rho_{i,i+1}$ and maximizations or minimizations procedures.

But such analyze is also trivially true for any property of the two spins, since they are completely determined by $\rho_{i,i+1}$, including the Bell measure. *Therefore $\mathcal{B}$ is, in principle, as good as any entanglement measure to signal a QPT.* But as in the case of entanglement accidental cancellations may also happen due to the complicated form $\mathcal{B}$ depends on $\rho_{i,i+1}$: it also involves the absolute value of $\rho_{i,i+1}$ and a maximization. Note that signaling the QPT is not the only interest when studying the behavior of entanglement or non-locality at QPT. One could also learn about the nature of the correlations involved in the QPT, as we will argue in the following when looking at the specific case of the XXZ model.

Given the general argument, we move to our results for the case of the XXZ model. The value of the Bell measurement, using Eq. (11), is shown in the upper curves of Fig. 4 for first (solid blue curve), second (dashed red curve) and third (doted yellow curve) neighbors. We observe that none of them violate the Bell inequality, despite being entangled. But lets first concentrate on the analytical properties of $\mathcal{B}$. As it may be expected from the arguments above, it is able to indicate the QPTs. Furthermore, *not only the first order QPT is revealed by $\mathcal{B}$, but also the Kosterlitz-Thouless QPT, which is neither indicated by the energy nor by the bipartite entanglement given in terms of the concurrence.* This can also be seen in Fig. 6 where we plot the derivatives of the Bell measurement $\mathcal{B}_1$ and the concurrence C_1 for nearest neighbors. It shows that while the derivative of both diverges at the first order quantum phase transition ($\Delta = -1$), only the derivative of the Bell measurement signal the infinite order quantum phase transition ($\Delta = 1$).

It is interesting to note that the success of $\mathcal{B}$ in revealing the KT-QPT comes from the maximization process, which is usually associated with negative results in the ability of entanglement to signal a QPT. More specifically, analyzing Eq. (11), we find out that while in the ferro and anti-ferromagnetic phase $|\langle\sigma_i^x\sigma_{i+r}^x\rangle| \leq |\langle\sigma_i^z\sigma_{i+r}^z\rangle|$ and $\mathcal{B}_r = 2\sqrt{\langle\sigma_i^x\sigma_{i+r}^x\rangle^2 + \langle\sigma_i^z\sigma_{i+r}^z\rangle^2}$, in the gapless phase $|\langle\sigma_i^x\sigma_{i+r}^x\rangle| > |\langle\sigma_i^z\sigma_{i+r}^z\rangle|$ and $\mathcal{B}_r = 2\sqrt{2\langle\sigma_i^x\sigma_{i+r}^x\rangle^2}$. On the other hand, the non-analytical behavior of $\mathcal{B}$ at the first order QPT does originate in $\rho_{i,i+r}$ or in e_0.

Just to contrast, we should mention that the non-analytical behavior of the concurrence does not come from the non-analyticities in e_0, but from the maximization involved in the concurrence. Note also that at the KT-QPT the first neighbor concurrence is maximum, while all the next neighbors are null almost in the whole phase. However, even though one can show that, in general, the concurrence may inherit the non-analytical behavior of e_0, it is not possible to show that it should be maximum at the critical point. Therefore, such a behavior, should not be an indication of a QPT and may be specific to the XXZ model; in fact it has been interpreted

as a consequence of the specific symmetries of the model (see Sec. IV-A-2 of [9]). It would be interest to know if the behavior of $\mathcal{B}$ at the KT-QPT is also only specific to this model.

Last, let us comment on the non-violation of the Bell inequality for nearest-neighbors, our third result. It is unexpectedly, since these spins are entangled, and not only slightly. They have a kind of hidden entanglement, similar to the one present in the Werner states, that is not revealed by the Bell inequality, being in this sense local. That entanglement may be relevant for quantum phase transitions has been suggested by many works [9]. *Our results complements such works, indicating that the kind of entanglement that is relevant for QPT is not trivial: it cannot be revealed by the Bell inequality.* Note that, one may argue that this should be expected since we are studying two particles in a huge chain in a pure highly entangled state. Thus, these two particles are in very mixed states close to the identity and should not violate the Bell inequality. But this argument also applies to entanglement: the two particles should not be entangled. In our case they are, and not slightly. In fact, despite even slight entangled states may violate Bell, the number of states violating Bell and the degree of violation increase with the amount of the entanglement [28]. We also observe that second and third neighbors do not violate Bell, but these are only weakly entangled in a tiny region of the phase diagram. Note that, even tough our states have a behavior similar to Werner states, they are not Werner states. Only at $\Delta = 1$ can our state be written in the form of a Werner state. Thus, these are a new class of entangled states, which do not violate the Bell Inequality.
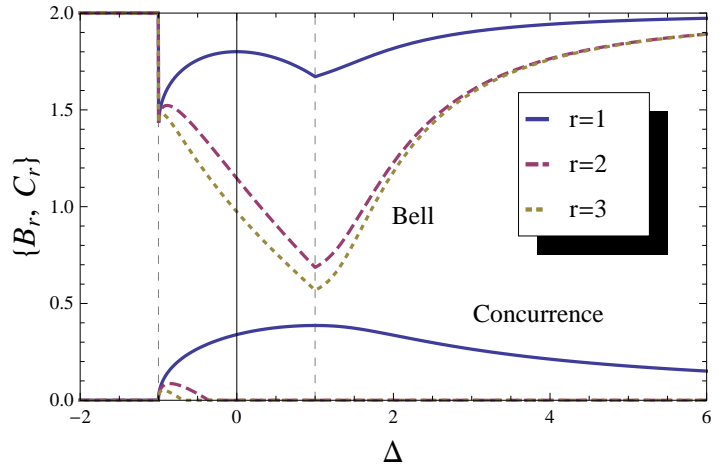

Figure 4: Bell measurement (three upper curves) and concurrence (three lower curves) for first, second and third neighbors of the XXZ model as a function of the anisotropy Δ. It can be seen that the Bell inequality is never violated, even when the two spins are entangled. While both the concurrence and the Bell measurement are able to signal the first order quantum phase transition at $\Delta = -1$, only the Bell measurement reveals the infinite order QPT at $\Delta = 1$.

Our results can be visualized geometrically in Fig. 5, where we have the parameter space of density matrices of two spin-$\frac{1}{2}$ particles with the symmetries of the XXZ Hamiltonian. Remember $\rho_{i,j}$ only depends on $\langle \sigma_i^x \sigma_j^x \rangle$ and $\langle \sigma_i^z \sigma_j^z \rangle$; Eq. (9). The greater triangle defines the physical states and the inner diamond the separable states (SEP). The two smaller triangles, inside and on the lower vertices of the greater, are the entangled states (ENT). The two smallest regions, also on the lower vertices of the greatest triangle, are the states violating Bell inequality (NL). The parallel lines are contour lines of the concurrence. We can see that it increases in the direction of the lower vertices of the greatest triangle. The contour lines of the Bell inequality are parallel to the lines defining the border of the region NL, but not show. We also plotted the "trajectory" of $\rho_{i,i+r}$ for $r = 1, 2$ and 3 as the parameter Δ is varied. For all the curves we marked fours points that corresponds to $\Delta = -1$ (full circle), -0.999 (square), 0 (triangle) and 1 (diamond). The whole ferromagnetic phase ($\Delta \leq -1$) is represented by the full circle. As we move from the ferromagnetic phase in the direction of the gapless ($-1 < \Delta < 1$) there is a jump at the point $\Delta = -1$. The state of $\rho_{i,i+1}$ (solid blue curve) and $\rho_{i,i+3}$ (dotted yellow) jumps through the left side, entering the entangled region, while $\rho_{i,i+2}$ (red dashed curve) jump to the entangled region through the right side. We can also observe that $\rho_{i,i+2}$ and $\rho_{i,i+3}$ barely enter the entangled region and go back to the separable one, while $\rho_{i,i+1}$ goes deeper in the entangled region and stays there in the whole gapless phase. The maximum value of the concurrence for $\rho_{i,i+1}$, at the critical point $\Delta = 1$, can be seen as the point where the trajectory tangencies a contour line of the concurrence. At this point the trajectory also touches a minimum of the Bell measurement, which happens due to the optimization procedure involved in its definition.

VI. CONCLUSION

We have studied non-locality using Bell inequality at quantum phase transitions. We first showed that *the Bell Inequality is, in principle, as good as any entanglement measurement to signal a* quantum phase transistion. Then, we studied the particular case of two spins in an one-dimensional spin-$\frac{1}{2}$ XXZ infinite chain at zero temperature and found that: i) *the Bell inequality is not only able to reveal the first order quantum phase transition, but also the Kosterlitz-Thouless quantum phase transition. This can not be indicated by the energy of the system nor by the bipartite entanglement given in terms of the concurrence.* ii) *the two spins, despite being entangled, never violate the Bell inequalities: their correlations can be then described by a realistic local theory.*

Our results suggest that the Bell inequality may contribute to the study of quantum phase transitions, since they are able to signal quantum phase transitions - and even the Kosterlitz-Thouless quantum phase transition,
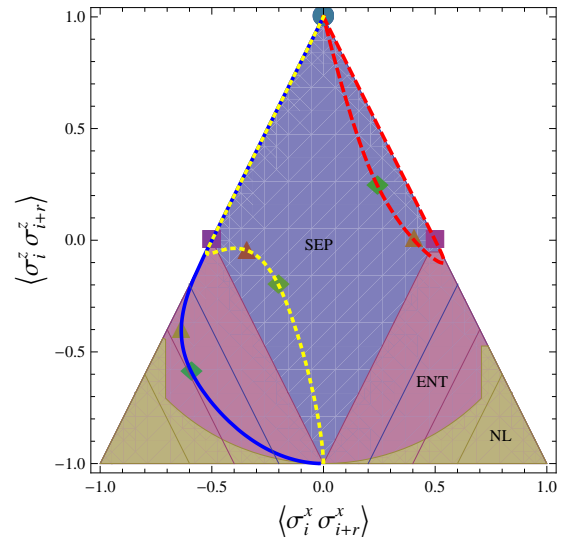

Figure 5: Parameter space of the reduced density matrix of two spins with the symmetries of the XXZ Hamiltonian. The greater triangle defines the physical states. The two smaller triangles, inside and on the lower vertices of the greater, are the entangled states (ENT). The two smallest regions, also on the lower vertices of the greatest triangle, are the states violating Bell inequality (NL). The curves are the "trajectory" of the ground state of the XXZ Hamiltonian as the parameter Δ is varied for $\rho_{i,i+1}$ (solid blue curve), $\rho_{i,i+2}$ (dashed red curve) and $\rho_{i,i+3}$ (dotted yellow curve). For all the curves we marked fours points that corresponds to $\Delta = -1$ (full circle), -0.999 (square), 0 (triangle) and 1 (diamond).
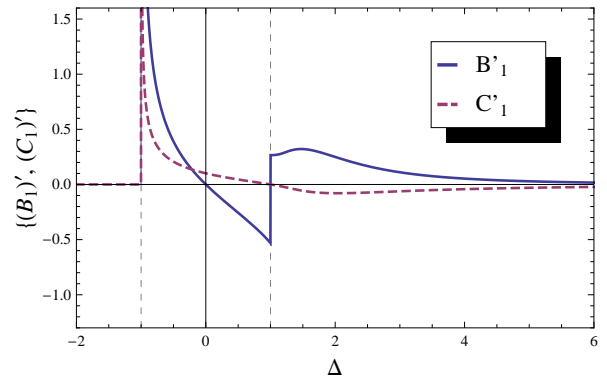

Figure 6: Derivative of the Bell measurement $\mathcal{B}_1$ and the concurrence C_1 in relation to Δ for nearest neighbors.

in our specific model. Furthermore, they may increase our understanding of the nature of the quantum correlations involved in quantum phase transitions. Again, in our specific model, it was shown that the type of entanglement which is relevant at the quantum phase transition is non-trivial, since it cannot be revealed by the Bell inequality. Therefore, Bell inequality constitute a different resource, other than entanglement, and could be an alternative and complementary way to characterize a quantum phase transition, maybe even infinite order

ones.

Our work gives information about the type of quantum correlation involved at the quantum phase transition of the XXZ model. To better characterize these quantum correlations, it would be interesting to study other models and more general Bell inequalities involving more measurement directions. The study of multipartite Bell inequalities is also of great interest, despite its technical difficulties. First, obtaining correlations among three or more spins in condensed matter systems suffering quantum phase transitions is not trivial. Second, there is no unique multipartite inequality, but many to be studied. However, a work on finite chain up to six spins was recently published[29].

Acknowledgments

[1] A. Einstein, B. Podolsky, and N. Rosen, Phys. Rev. **47**, 777 (1935).

[2] J. S. Bell, Physics **1**, 195 (1964).

[3] R. F. Werner, Phys. Rev. A **40**, 4277 (1989).

[4] A. Osterloh, L. Amico, G. Falci, and R. Fazio, Nature **416**, 608 (2002).

[5] Tobias J. Osborne, and Michael A. Nielsen, Phys. Rev. A **66**, 032110 (2002).

[6] L.-A. Wu, M. S. Sarandy, and D. A. Lidar, Phys. Rev. Lett. **93**, 250404 (2004).

[7] L.-A. Wu, M. S. Sarandy, D. A. Lidar, and L. J. Sham, Phys. Rev. A **74**, 052335 (2006).

[8] M.-F. Yang, Phys. Rev. A **71**, 030302(R) (2005).

[9] Luigi Amico, Rosario Fazio, Andreas Osterloh and Vlatko Vedral, Rev. Mod. Phys. **80**, 517 (2008).

[10] J. Batle and M. Casas, Phys. Rev. A **82**, 062101 (2010).

[11] N. Gisin, Phys. Lett. A **154**, 201 (1991).

[12] Sandu Popescu, Phys. Rev. Lett. **74**, 2619 (1995).

[13] Daniel Collins and Nicolas Gisin, J. Phys. A: Math. Gen. **37**, 1775 (2004).

[14] Yeong-Cherng Liang, PhD Thesis, arXiv:0810.5400v1 [quant-ph].

[15] A. A. Methot, V. Scarani, Quantum Information and Computation **7**, 1 (2007) 157-170. arXiv:quant-ph/0601210v1.

[16] M. S. Sarandy, Phy. Rev. A **80**, 022108 (2009).

[17] T. Werlang, C. Trippe, G. A. P. Ribeiro, and Gustavo Rigolin, Phys. Rev. Lett. **105**, 095702 (2010).

[18] R. Dillenschneider, Phys. Rev. B **78**, 224413 (2008).

[19] C. N. Yang and C. P. Yang, Phys. Rev. **150**, 1 (1966) 321-327; **150**, 1 (1966) 327-339.

[20] M. Shiroishi and M. Takahashi, J. Phys. Soc. Jpn. **74** (2005) Suppl. pp. 47–52.

[21] Thiago R. de Oliveira, Gustavo Rigolin, Marcos C. de Oliveira, and E. Miranda, Phys. Rev. A **77**, 032325 (2008).

[22] Andreas Osterloh, Guillaume Palacios, and Simone Montangero, Phys. Rev. Lett. **97**, 257201 (2006).

[23] R. Horodecki, P. Horodecki, M. Horodecki, Phys. Lett. A **200** (1995) 340-344.

[24] Ryszard Horodecki, Pawel Horodecki, Michal Horodecki, and Karol Horodecki, Rev. Mod. Phys. **81**, 865 (2009).

[25] O. F. Syljuasen, Phys. Rev. A **68**, 060301(R) (2003).

[26] Shi-Jian Gu, Hai-Qing Lin, and You-Quan Li, Phys. Rev. A 68, 042330 (2003).

[27] Thiago R. de Oliveira, Gustavo Rigolin, Marcos C. de Oliveira, and Eduardo Miranda, Phys. Rev. Lett. 98, 079902 (2007).

[28] Frank Verstraete and Michael M. Wolf, Phys. Rev. Lett. 89, 170401 (2002).

[29] Steve Campbell and Mauro Paternostro, Phys. Rev. A 82, 042324 (2010).

[30] Ferdi Altintas, Resul Eryigit, arXiv:1202.1495v1 [quant-ph] (2012).

[31] Dong-Ling Deng, Chunfeng Wu, Jing-Ling Chen, Shi-Jian Gu, Sixia Yu, C. H. Oh, arXiv:1111.4341v1 [quant-ph] (2011).

[32] X. Wang and P. Zanardi, Phys. Lett. A **301** (2002) 1–6.

[33] Clauser J. F., Horne M. A., Shimony A. and Holt R. A., Phys. Rev. Lett. **23**, 880 (1969).

[34] G. Kato, M. Shiroishi, M. Takahashi and K. Sakai, J. Phys. A: Math. Gen. **37** (2004) 5097–5123.

[35] After finishing this work we become aware of two related studies [30, 31]. For the sake of completeness, we should also mention the study of Bell Inequality for only two spins interacting via Heisenberg coupling, and not at a quantum phase transition [32].

[36] In this paper we used the Bell-CHSH inequality, so where we see Bell inequality we read Bell-CHSH inequality. Actually, the inequality derived by Bell [2] was a little different and not suitable to experimental verification, while the inequality above was written by Clauser, Horne, Shimony and Holt [33], hence CHSH inequality, and is the one usually tested experimentally.

[37] Note that, if a given state does not violate the inequality above, we can only say that this specific combination of correlations can be described by a realistic local theory. One may still find another inequality violated by the state. Fortunately, for 2 qubits, and only 2 measurement directions per particle, it is known that the CHSH inequality is complete: a state satisfying it, will also satisfy any other inequality. But we can only really state that a state is local if it does not violate any inequality for any kind of experiment; measures in any number of directions, for example. Here, we will not be so accurate and may use the term "local" for states which do not violate the CHSH inequality.

[38] There are some typos in equations (19) and (20) from

[20]. In (19) we only need to sum a $-\frac{c_1}{\pi s_1}\zeta_\nu$. In (20) we need to go to [34] (note that equation (5.4) has the same typo) and use equations (5.10), (B.11) and (B.12) to calculate and find the typo in $\langle \sigma_i^x \sigma_{i+3}^x \rangle$